Ethyl 3-hydroxybenzoate

7781-98-8 | DTXSID10228435

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 2.17e-04 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.80e-01

Confidence level: 4.54e-01

Nearest Neighbors from the Training Set

Image not found
Isopentyl benzoate
Measured: 5.90e-06
Predicted: 4.01e-02

Image not found
Butyl phenyl ether
Measured: 1.08e-03
Predicted: 5.92e-01

Image not found
Pyrethrin II
Measured: 1.04e-05
Predicted: 3.95e-07

Image not found
2-Methoxyprop-1-ene
Measured: 8.46e-02
Predicted: 474